

A method to estimate the energy distribution during the confined comminution of granular materials

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ABSTRACT: During the confined comminution of granular materials, the work input is transformed into elastic energy stored in the grains, breakage energy used to generate new surfaces, energy dissipated by friction between grains in contact, and redistribution energy dissipated by the relative movement of crushed fragments. We assume that the expression of Particle Size Distribution (PSD) in a crushed sample is a function of a fractal distribution and a uniform distribution. This allows calculating the breakage parameter, the increase of surface energy, and finally the energy dissipated by breakage. By summing the contact energy at all the contacts within a sample, we calculate the elastic energy stored. The calculation of friction-dissipated energy requires calculating relative movements of contacts, which are highly unpredictable especially when crushing is involved. Thus we include the dissipation that results from the relative displacement of grains in contact (including both crushed fragments and surrounding intact grains) in the friction-dissipated energy. We obtain the friction-dissipated energy by subtracting the elastic energy stored in the grains and the breakage energy from the input energy. The results show that the energy distribution is stress sensitive and changes a lot with the increase of compressive stress. Energy dissipation by friction plays a major role during confined comminution.

1. INTRODUCTION

Quasi-static confined comminution is a mechanical process in which particle sizes decrease due to high compressive stress. This method is encountered in civil engineering, powder technology and the mineral industry. During this comminution, the total input energy (δW) at the boundary is transformed into elastic energy stored in grains, breakage energy, friction energy and redistribution energy - the dissipation of the kinetic energy triggered by crushing (McDowell, 1996; Nguyen and Einav, 2009; Russell and Einav, 2013). The complete energy balance equation is given by (Russell, 2011):

$$\delta W = \delta \Psi + \delta \Phi_p + \delta \Phi_s + \delta \Phi_{redist} \quad (1)$$

where $\delta \Psi$, $\delta \Phi_p$, $\delta \Phi_s$ and $\delta \Phi_{redist}$ represent elastic energy, friction dissipation, breakage energy and redistribution energy, respectively.

The ratios among the different energy components are still unknown. Based on the conventional $p-q$ notations in soil mechanics, the following work balance equation was proposed (McDowell, 1996):

$$pd\varepsilon_v^p + qd\varepsilon_s^p = Mp|d\varepsilon_s^p| + \Gamma^* dS. \quad (2)$$

The left hand side in Eq. (2) is the increment of plastic work put into the system per unit volume, and the right

hand side terms represent the friction dissipation and breakage energy. Initially, the parameter Γ^* , which is the fracture surface energy, was not fully validated and calibrated. Later the parameter $R = \delta \Phi_{redist} / \delta \Phi_s$ was defined as the ratio of redistribution energy and breakage energy (Russell, 2011). Based on a calibration against two oedometric tests performed on silica sands, the value of R was found to be between 13 and 16. None of the studies considers the effect of the compression stress on energy distribution. In order to address this problem, a series of uniaxial compression tests were conducted with crushable sand of uniform distribution (Ovalle, 2013). The results showed that the surface fracture energy is indeed stress dependent and that its influence becomes less significant at high stresses. However, the comparison of redistribution energy with pure breakage or friction energy was not discussed.

In this paper, we analyze the role of different energy components during confined comminution and particularly their dependence on the compression stress. To this aim, we use both empirical and numerical methods to calculate the different energy components. The dissipation of redistribution energy is triggered by breakage but increases due to the production of kinetic energy and friction energy. The kinetic component is small in the case of quasi-static comminution. Thus, by contrast with previous studies, we include the

redistribution energy into the friction dissipation and Eq. (1) becomes

$$\delta W = \delta \Psi + \delta \Phi_p + \delta \Phi_s. \quad (3)$$

The total input energy is calculated from the force-displacement curve obtained in experiments or simulations. The breakage energy is the product of a constant that represents the material free surface energy by the new surface area created by particle breakage. In order to calculate the area of the new surfaces, we postulate that the Particle Size Distribution (PSD) of the crushed sample is a function of the ultimate fractal distribution and a uniform distribution with fixed d_{\max} and varying d_{\min} . The relative breakage is calculated in the same way as in (Einav, 2007), with PSDs that fit published compression experiments even at low stress (i.e. with low breakage). The relative breakage parameter allows updating the PSD of the crushed sample and calculating the area of the new grain surfaces created by breakage. The elastic energy is calculated by the Discrete Element Method (DEM). Simulations of uniaxial compression tests are conducted with the calculated PSD, and the elastic energy stored in the particles of the crushed sample is calculated by summing both normal and shear energy stored at particle contacts. With the total input energy, elastic energy and breakage energy, on Eq. (3) allows getting the energy dissipated by friction.

2. ENERGY CALCULATION OF UNIAXIAL COMPRESSION TESTS

In this section, we present the method to calculate the energy components involved in Eq. (3). We used results of uniaxial compression tests performed on cylindrical samples of dry sand (Ovalle, 2013). Samples were 19mm in height and 70 mm in diameter with an initial uniform PSD with grain size between 2.0 and 2.5mm. We used data from the four dry tests, with maximum compressive stresses of 0.4MPa, 0.6MPa, 2.1MPa and 2.1MPa.

2.1. Total Input Energy

In the uniaxial compression test, the loading platen is the only source of energy input, which has the form:

$$\delta W = F * \delta S \quad (4)$$

where F is the loading force and δS is the increment of displacement. Experimental results for the four tests (Test 1 to Test 4) are shown in Fig. 1: the total input work is the area below each curve. Note that the four samples had different initial void ratios, thus different macroscopic stiffness in Fig. 1.

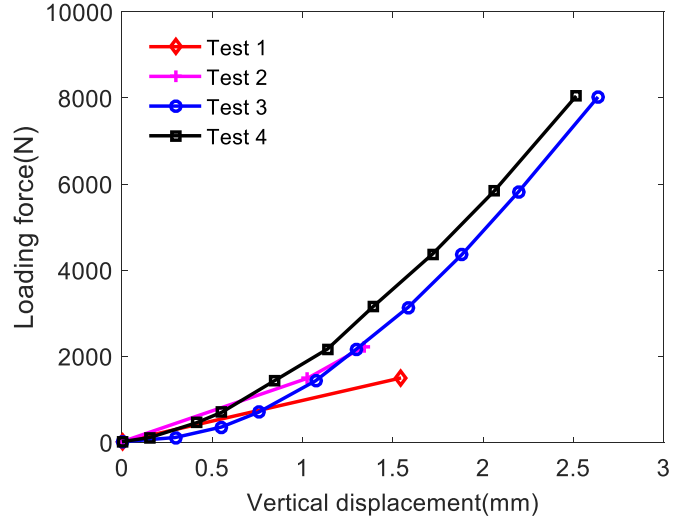


Fig. 1. Load-displacement curve of uniaxial compression tests performed on crushable sand samples (Ovalle, 2013)

2.2. Breakage Energy

The breakage energy is the energy needed to create new surfaces. Therefore, it is the product of surface free energy by the grain surface area created by breakage. During compression, particles break continuously due to the increasing contact forces. As a result, the number of fines as well as the total surface area of fragments increase with the compressive stress. At extremely high stress, the PSD reaches an ultimate PSD, which is often assumed to be fractal, with an expression of the form $F_u(d) = (d/d_M)^{3-\alpha}$ (where α is the fractal dimension and d_M is the maximum particle size).

Since the surface free energy is a material constant, it becomes important to have an appropriate estimation of the current PSD to calculate the breakage energy. We propose to model the current PSD of the crushed sample as follows:

$$F_c(d) = aF_u(d) + (1-a)F_b(d) \quad (5)$$

where $F_u(d)$ is the ultimate PSD and $F_b(d)$ is a uniform distribution between a fitting parameter d_b and d_M . This equation originates from the definition of the relative breakage B_r parameter (Einav, 2007), in which $F_0(d)$ is replaced with a uniform distribution $F_b(d)$. The model in Eq.(5) is fitted to the experimental PSDs (Fig.2). The fitting curve with Relative Breakage is also shown for Test 1. It is clear that PSDs expressed with Eqn. (5) can better capture the breakage of large particles: the PSD obtained from the definition of the relative breakage parameter is the same as the initial PSD for larger particles. Table 1 shows the calibrated parameters a and d_b for Tests 1-4.

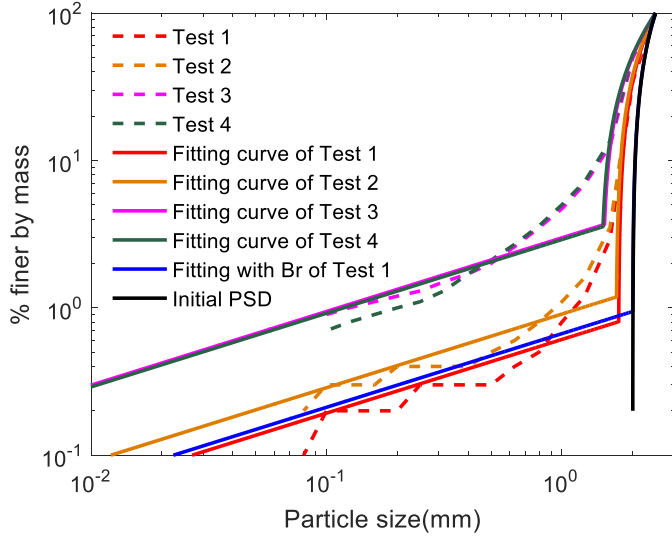


Fig. 2. Particle size distributions and their best fit according to Eq.(5)

Table 1. Parameters a and d_b for uniaxial compression tests

Test #	a	d_b
1	0.0096	1.744
2	0.0143	1.707
3	0.0472	1.518
4	0.0459	1.495

Now consider for a small particle size comprised between d_{im} and d_{iM} . The mass of particles of that size is $M_i = M_T (F_c(d_{iM}) - F_c(d_{im}))$, where M_T is the sample mass, which remains constant. Then the number of particles in this fraction is given by $N_i = M_i / (\rho V(d))$. Now we can calculate the surface area in this fraction as $S_i = N_i s(d)$ where $s(d)$ is the surface of a sphere of diameter d . The total surface area is summation of the areas of spheres of all size fractions.

2.3. Elastic Energy

Elastic energy is stored at the contacts between grains. Therefore, with the assumption of constant particle stiffness, the elastic energy can be calculated as:

$$\Psi = 2 \sum_{i=1}^c \frac{F_{ci}^2}{2k} \quad (6)$$

where c is the number of total contacts, F_{ic} is contact force and k is the stiffness of the particle (normal or shear stiffness, depending on the orientation of the contact force). Note that each contact contains two particles, so the elastic energy is multiplied by 2.

The elastic energy is calculated by using the DEM software PFC3D4.0. DEM samples with PSDs shown in Fig. 2 were generated. The samples had the same sizes,

weight and densities as in the experiments. We use the same stiffness for normal and shear deformation for all the particles, and assume a linear relationship between force and contact displacement. Fig. 3 shows the sample used for Test 2, before compression. A summary of the parameters used in the simulation is reported in Table 2.

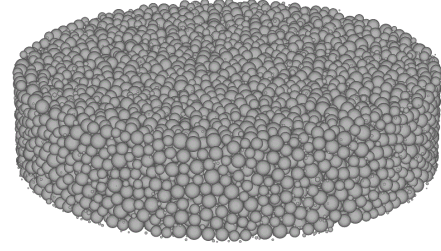


Fig. 3. DEM sample used to simulate the uniaxial compression test #2

Table 2. Parameters used in DEM simulations

Input parameter	Value
Density of sphere: kg/m ³	2750
Normal stiffness: N/m	1.5×10^6
Shear stiffness: N/m	1.5×10^6
Frictional coefficient	0.5
Number of particles (Test 1-Test 4)	8000-30800

The total number of particles in Tests 3 and 4 was about two million, which is highly computationally expensive. According the PSDs, particles under 0.1mm in size account for more than 95% of the total number of particles but for less than 1% of the sample weight. Since larger particle tends to store more energy, we removed particles with diameter less than 0.1mm from the model to conduct the simulation.

After generating the sample, we imposed a controlled velocity on the top platen to apply the uniaxial compression force. The force was continuously monitored during the loading process. When the force reached the value imposed in the experiment, we stopped loading and we calculated the total elastic energy stored in the sample. Note that it is not necessary to consider the crushing of particles here because the goal for this simulation is only to obtain the elastic energy for a specific PSD under a given compression stress.

2.4. Friction Energy

Sections 2.1 to 2.3 explain how to obtain the input energy, the breakage energy and the elastic energy. Therefore, the friction energy can be directly calculated by subtracting the elastic energy and the breakage energy from the total input energy according to Eq. (3). All the components of energy can now be determined. Next, we discuss the relative importance of energy dissipation by breakage and friction.

3. RESULTS

The initial void ratio, compressive force and increase of specific surface are reported in Table 3 for the four tests. As expected, the specific surface increases with the loading force. The relationship between the two is linear, see Fig. 4. The value of the surface free energy for sand ranges from 0.3 to 1.0 J/m² depending on the environmental conditions (Friedman et al., 1972). In this research, we use 0.5 J/m² to calculate the breakage energy. Results are shown in Table 5.

Table 3. Material surface increase during the compression tests

Test #	Initial Void Ratio	Maximum Force(N)	Surface Increase (mm ² /g)
1	1.066	1499.63	2224.84
2	1.015	2227.53	2537.18
3	1.015	8023.61	4195.36
4	0.990	8046.79	4280.13

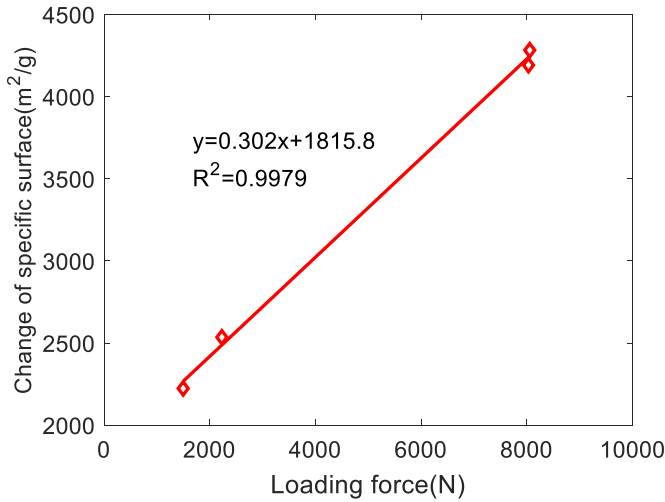


Fig. 4. Relationship between loading force and surface increase

By integrating the Load-displacement curve in Fig. 1, we obtain the input energy of Tests 1-4. The breakage energy is calculated from the area of new surfaces created. For each test, we conducted 3 DEM simulations to calculate the elastic energy, and the simulation results are shown in Table 4. The increase of elastic energy with loading force is obvious.

Table 4 Elastic energy calculated by DEM

Test #	Model 1 (mJ/g)	Model 2 (mJ/g)	Model 3 (mJ/g)	Average (mJ/g)
1	1.56	1.48	1.58	1.54
2	2.31	2.28	2.31	2.30
3	10.38	10.51	10.88	10.60
4	13.39	13.31	13.35	13.35

The friction dissipation energy is calculated by subtracting the elastic energy and the breakage energy

from the total work input. A summary of the results on energy distribution is provided in Table 5.

Table 5. Energy distribution during Tests 1-4

Test #	Input Energy (mJ/g)	Breakage Energy (mJ/g)	Elastic Energy (mJ/g)	Friction Dissipation (mJ/g)
1	23.82	1.54	1.10	21.18
2	29.97	2.30	1.25	26.42
3	74.67	10.60	2.10	61.98
4	77.37	13.35	2.15	61.87

In order to see the role of each energy component during the comminution process, we normalized the data in Table 5 with the corresponding input energy, and the results are shown in Fig. 5.

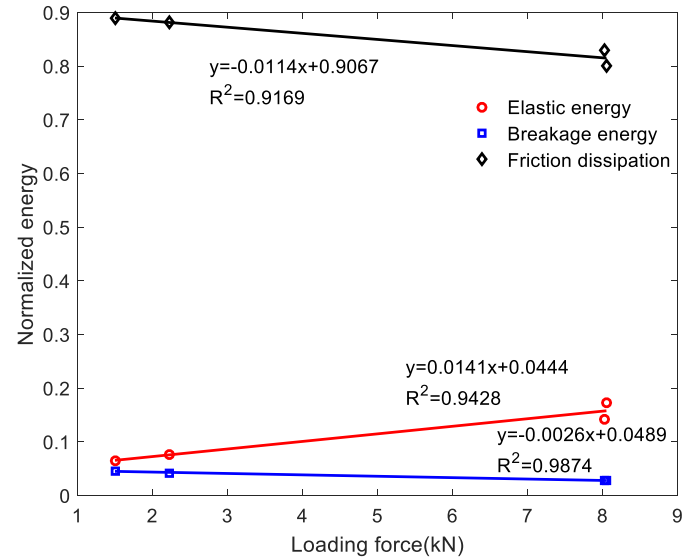


Fig. 5. Evolution of normalized energy components

Fig. 5 shows that for all the 4 tests, more than 80% of the total energy is dissipated by friction between particles. Between 8% and 20% of the work input is transformed into elastic energy. The breakage energy is less than 5%. Energy dissipation by friction and breakage increase continuously, but in relative proportions, the friction and breakage energy components decrease compared to the elastic energy stored in the sample. Therefore, at higher stress more input energy is transformed into elastic energy.

4. CONCLUSION

In this paper, we propose a method to analyze the energy distribution during confined comminution. We consider that the redistribution energy is part of the energy dissipated by friction. The work input is calculated by integrating force-displacement curves obtained experimentally by other authors. The breakage energy is determined by assuming the form of the expression of the current PSD of the crushed sample. The elastic

energy stored in the sample is calculated by computing the work done by contact forces in a DEM sample that has the same PSD as the current PSD obtained experimentally. The results indicate that all components of energy increase with the loading force (input energy). The relationship between the change of particle surface area and the loading force is linear. The energy dissipated by friction is 8 times (respectively 15 times) larger than the elastic energy (respectively than the breakage energy). Results are conform to previous experimental and numerical studies. The breakage energy accounts for less than 5% of the total input energy, and this fraction actually decreases as the compression force increases. The percentage of elastic energy stored in the sample increases with the loading force, while the percentage of energy dissipated by friction and breakage do not. The elastic plays a more important role when the axial loading force is high. This research is expected to increase the fundamental understanding of microstructure changes during confined comminution and to provide a concrete foundation to establish energy based constitutive relationships for granular materials.

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